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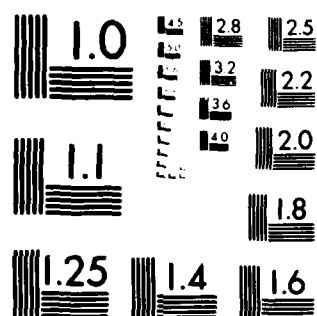
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LARGE SCALE GEODETIC LEAST SQUARES ADJUSTMENT BY
DISSECTION AND ORTHOGONAL DECOMPOSITION

by

Gene H. Golub
Robert J. Plemmons

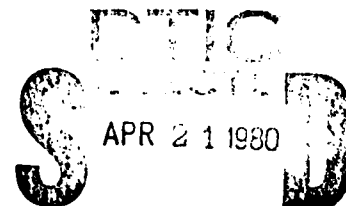
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LARGE SCALE GEODETIC LEAST SQUARES ADJUSTMENT BY
DISSECTION AND ORTHOGONAL DECOMPOSITION

by

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ABSTRACT

Very large scale matrix problems currently arise in the context of accurately computing the coordinates of points on the surface of the earth. Here geodesists adjust the approximate values of these coordinates by computing least squares solutions to large sparse systems of equations which result from relating the coordinates to certain observations such as distances or angles between points. The purpose of this paper is to suggest an alternative to the formation and solution of the normal equations for these least squares adjustment problems. In particular, it is shown how a block-orthogonal decomposition method can be used in conjunction with a nested dissection scheme to produce an algorithm for solving such problems which combines efficient data management with numerical stability. As an indication of the magnitude that these least squares adjustment problems can sometimes attain, the forthcoming readjustment of the North American Datum in 1983 by the National Geodetic Survey is discussed. Here it becomes necessary to linearize and solve an overdetermined system of approximately 6,000,000 equations in 400,000 unknowns - a truly large-scale matrix problem.

1. Introduction.

Recent technological advances have made possible the collection of vast amounts of raw data describing certain physical phenomena. As a result, the sheer volume of the data has necessitated the development of new elaborate schemes for processing and interpreting it in detail. An example is in the adjustment of geodetic data.

Geodesy is the branch of applied mathematics which is concerned with the determination of the size and shape of the earth, the directions of lines and the coordinates of stations or points on the earth's surface. Applications of this science include mapping and charting, missile and space operations, earthquake prediction, and navigation. The current use of electronic distance measuring equipment and one-second theodolites for angle measurements by almost all surveyors necessitates modern adjustment procedures to guard against the possibility of blunders as well as to obtain a better estimate of the unknown quantities being measured. The number of observations is always larger than the minimum required to determine the unknowns. The relationships among the unknown quantities and the observations lead to an overdetermined system of nonlinear equations. The measurements are then usually adjusted in the sense of least squares by computing the least squares solution to a linearized form of the system that is not rank deficient.

In general, a geodetical position network is a mathematical model consisting of several mesh-points or geodetic stations, with unknown positions over a reference surface or in three-dimensional space. These stations are normally connected by lines, each representing one or more observations

involving the two stations terminating the line. The observations may be angles or distances, and thus they lead to nonlinear equations involving, for example, trigonometric identities and distance formulas relating the unknown coordinates. Each equation typically involves only a small number of unknowns.

As an illustration of the sheer magnitude that some of these problems can attain, we mention the readjustment of the North American Datum - a network of reference points on the North American continent whose longitudes, latitudes and, in some cases, altitudes must be known to an accuracy of a few centimeters. This ten-year project by the U.S. National Geodetic Survey is expected to be completed by 1983. The readjusted network with very accurate coordinates is necessary to regional planners, engineers and surveyors, who need accurate reference points to make maps and specify boundary lines; to navigators; to road builders; and to energy resource developers and distributors. Very briefly, the problem is to use some 6,000,000 observations relating the positions of approximately 200,000 stations (400,000 unknowns) in order to readjust the tabulated values for their latitudes and longitudes. This leads to one of the largest single computational efforts ever attempted - that of computing a least squares solution of a very sparse system of 6,000,000 nonlinear equations in 400,000 unknowns. This problem is described in detail by Meissl [1979], by Avila and Tomlin [1979], and from a layman's point of view by Kolata [1978] in Science.

In general then, geodetical network adjustment problems can lead (after linearization) to a very large sparse overdetermined system of m linear equations in n unknowns

$$Ax \approx b \quad (1.1)$$

where the matrix A , called the observation matrix, has full column rank. The least squares solution to (1.1) is then the unique solution to the problem:

$$\min_x \|b - Ax\|_2.$$

An equivalent formulation of the problem is the following: one seeks to determine vectors y and r such that $r + Ay = b$ and $A^t r = 0$. The least squares solution to (1.1) is then the unique solution y to the nonsingular system of normal equations

$$A^t A y = A^t b. \quad (1.2)$$

The linear system of equations (1.2) is usually solved by computing the Cholesky factorization

$$A^t A = R^t R, \quad R = \begin{bmatrix} & & \\ & & \\ 0 & & \end{bmatrix}$$

and then solving $R^t w = A^t b$ by forward substitution and $Ry = w$ by back substitution. The upper triangular matrix R is called the Cholesky factor of A .

Most algorithms for solving geodetic least squares adjustment problems (see Ashkenazi [1971], Bomford [1971], Meissl [1979] or Avila and Tomlin [1979]) typically involve the formation and solution of some (weighted) form of the normal equations (1.2). But because of the size of these problems and the high degree of accuracy desired in the coordinates, it

is important that particular attention be paid to sparsity considerations when forming $A^t A$ as well as to the numerical stability of the algorithm being used. It is generally agreed in modern numerical analysis theory (see Golub [1965], Lawson and Hanson [1974] or Stewart [1978]) that orthogonal decomposition methods applied directly to the matrix A in (1.1) are preferable to the calculation of the normal equations whenever numerical stability is important. Since A has full column rank, the Cholesky factor, R , of A can be computed by

$$Q^t A = \begin{bmatrix} R \\ 0 \end{bmatrix}, \quad Q^t Q = I, \quad R = \begin{bmatrix} \text{upper triangular} \\ 0 \end{bmatrix} \quad (1.3)$$

where the orthogonal matrix Q results from a finite sequence of orthogonal transformations, such as Householder reflections or Givens rotations, chosen to reduce A to upper triangular form.

Since A has the orthogonal decomposition $A = Q \begin{bmatrix} R \\ 0 \end{bmatrix}$, then defining $Q^t b = \begin{bmatrix} c \\ d \end{bmatrix}$, where c is an n -vector, the least squares solution y to (1.1) is obtained by solving $Ry = c$ by back substitution. The greater numerical stability of the orthogonal decomposition method results from the fact that the spectral condition number of $A^t A$ in the normal equations (1.2) is the square of the spectral condition number of A . The orthogonal decomposition method (1.3) has other advantages, including the ease with which updating and downdating of the system (1.1) can be accomplished, and the fact that possible fill-in in forming the normal equations is avoided (see, for example, Björck [1976]).

However, orthogonal decomposition techniques for solving large sparse least squares problems such as those in geodesy have generally been avoided, in part because of tradition and in part because of the lack of effective means for preserving sparsity and for managing the data.

Modern techniques for solving large scale geodetic adjustment problems have involved the use of a natural form of nested dissection, called Helmert blocking by geodesists, to partition and solve the normal equations (1.2). Such techniques are described in detail in Avila and Tomlin [1979], in Hanson [1978], and in Meissl [1979] where error analyses are given.

The purpose of this paper is to develop an alternative to the formation and solution of the normal equations in geodetic adjustments. We show how the orthogonal decomposition method can be combined with a nested dissection scheme to produce an algorithm for solving such problems that combines efficient data management with numerical stability.

In subsequent sections the adjustment problem is formulated, and it is shown how nested dissection leads to an observation matrix A in (1.1) of the special partitioned form

$$A = \left[\begin{array}{c|c} \begin{array}{c} \text{[shaded box]} \\ \text{[shaded box]} \\ \vdots \\ \text{[shaded box]} \end{array} & \text{[large shaded box]} \end{array} \right] \quad (1.4)$$

where the diagonal blocks are normally rectangular and dense and where the large block on the right-hand side is normally sparse with a very special structure. The form (1.4) is analyzed and a block-orthogonal decomposition scheme is described. The final section contains some remarks on the advantages of the approach given in this paper and relates the concepts mentioned here to further applications. Numerical experiments and comparisons are given elsewhere in Golub and Plemmons [1980].

2. Geodetic Adjustments.

In this paper we consider geodetical position networks consisting of mesh-points, called stations, on a two-dimensional reference surface. Associated with each station there are two coordinates. A line connecting two stations is roughly used to indicate that the coordinates are coupled by one or more physical observations. Thus the coordinates are related in some equation that may involve, for example, distance formulas or trigonometric identities relating angle observations. An example of such a network appears in Figure 1.

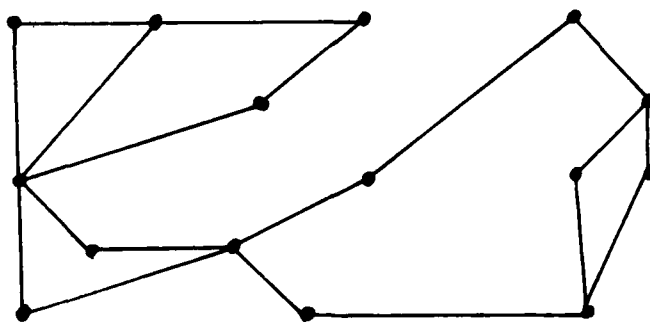


FIGURE 1

A 15 station network.

More precisely, one considers a coordinate system for the earth and seeks to locate the stations exactly, relative to that system. Usually coordinates are chosen from a rectangular geocentric system (see Bomford [1971]). Furthermore, a reference ellipsoid of revolution is chosen in this set of coordinates and the projection of each station onto this ellipsoid determines the latitude and longitude of that station.

As indicated initially in Section 1, the relationships among the coordinates of the stations in the geodetic network lead to an overdetermined system of nonlinear equations

$$F(p) = q \quad (2.1)$$

where

p = vector of unknown coordinates, and

q = vector of observations.

The components of $F(p)$ represent the equations that express the relationships among the unknown parameters and the observations or measurements made, for example, by surveyors.

A common procedure for solving the overdetermined system (2.1) is the method of variation of parameters. (This is generally called the Gauss-Newton nonlinear least squares algorithm in the mathematical literature). Approximate coordinates are known a priori. Let

p^0 = current vector of approximate coordinates.

Then if F has a Taylor's series expansion about p^0 , there follows the relationship

$$F(p) = F(p^0) + F'(p^0)(p - p^0) + \dots$$

where $F'(p^0)$ denotes the Jacobian of F at p^0 . Then taking

$$A = F'(p^0)$$

$$x = p - p^0$$

$$b = q - F(p^0)$$

and truncating the series after 2 terms, one seeks the solution to:

$$\min_x \|b - Ax\|_2 \quad (2.2)$$

The least squares solution y then represents the correction to p^0 . That is, one takes

$$p^1 = p^0 + y$$

as the next approximation to p . The process is, of course, iterative and one can use p^1 to compute a further approximation to p . Normally, the initial coordinates have sufficient accuracy for convergence of the method, but the number of iterations is often limited by the sheer magnitude of the computations. Thus a very accurate approximation to y is desired.

Actually, the equations are usually weighted by use of some positive diagonal matrix W , where the weights are chosen to reflect the confidence in the observations: thus (2.2) becomes

$$\min_x \|W^{\frac{1}{2}}b - W^{\frac{1}{2}}Ax\|_2$$

For simplicity, we will use (2.2) in the analysis to follow. The procedure

we discuss, however, will not be complicated by the weights.

Due to the sheer volume of the data to be processed in many adjustment problems, it is imperative to organize the data in such a way that the problem can be broken down into meaningful mathematical subproblems which are connected in a well-defined way. The total problem is then attacked by "solving" the subproblems in a topological sequence. This "substructuring" or "dissection" process has been used by geodesists for almost a century. The method they have employed dates back to Helmert [1880] and is known as Helmert blocking (see Wolf [1978] for a historical discussion).

In Helmert blocking, geographical boundaries for the region in question are chosen to partition it into regional blocks. This technique orders the stations appropriately in order to establish barriers which divide the network into blocks. The barriers are chosen so that the interior stations in one block are not coupled by observations to interior stations in any other block. These interior blocks are separated by sets of junction stations which are coupled by observations to stations in more than one block. An example of such a partitioning of the geodetic network in Figure 1 to one level of Helmert blocking is provided in Figure 2. Here the circled nodes represent the junction stations chosen for this example.

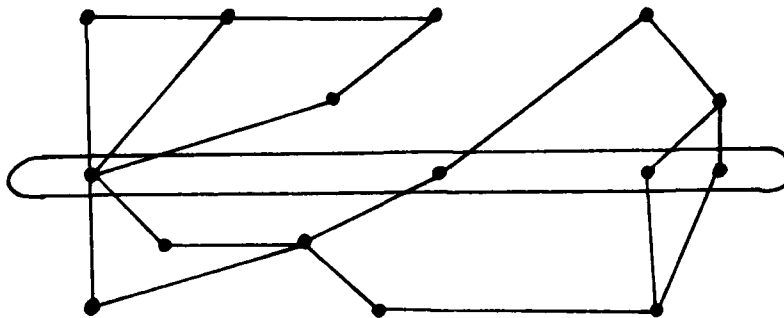


FIGURE 2

One level of Helmert blocking.

The particular form of Helmert blocking we will use here is the same as that used by Avila and Tomlin [1979] for partitioning the normal equations. That procedure, in certain respects, is a variation of the nested dissection method developed by George [1973], [1977]; George and Lui [1978]; and George, Poole and Voight [1978]. The primary emphasis of the nested dissection strategy has been on solving symmetric positive-definite systems of linear equations associated with finite element schemes for partial differential equations. There, the finite element nodes are ordered in such a way that the element matrix B is permuted into the block partitioned form

$$B = \left[\begin{array}{cccccc|c} B_1 & 0 & . & . & . & 0 & \\ 0 & B_2 & . & . & . & 0 & \\ . & . & . & . & . & . & \\ . & . & . & . & . & . & \\ . & . & . & . & . & . & \\ 0 & 0 & . & . & . & B_k & \\ \hline & & & & & & C^t \\ \hline & & & & & & D \end{array} \right]$$

where the diagonal blocks are square.

In our case we use the following dissection strategy in order to permute the observation matrix A into the partitioned form (1.4) Our procedure will be called nested bisection.

Given a geodetical position network on a geographical region R , first pick a latitude so that approximately one-half of all the stations lie south of this latitude. This forms two blocks of interior stations and one block of separator or junction stations and contributes one level of nested bisection (see Figure 3).

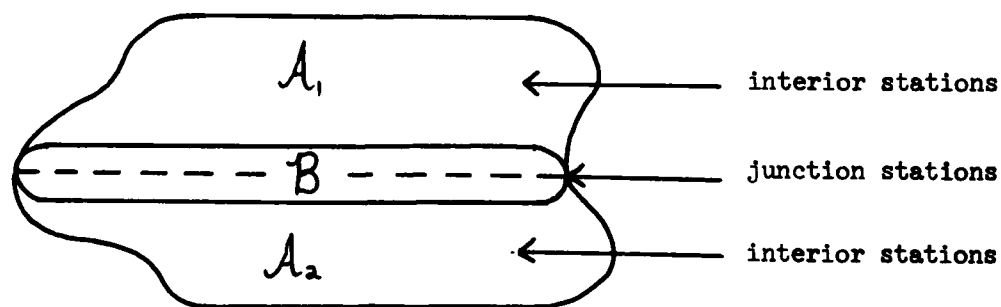


FIGURE 3

One level of nested bisection.

Now order the stations in R so that those in the interior regions \mathcal{A}_1 appear first, those in the interior region \mathcal{A}_2 appear second, and those in the junction region B appear last; order the observations (i.e., order the equations), so that those involving stations in \mathcal{A}_1 come first, followed by those involving stations in \mathcal{A}_2 ; then the observation matrix A can be assembled into the block-partitioned form:

$$A = \begin{bmatrix} \text{shaded } A_1 & & \text{shaded } B \\ & \text{shaded } A_2 & \text{shaded } B \end{bmatrix}$$

Thus A can be expressed in the block-partitioned form:

$$A = \begin{bmatrix} A_1 & 0 & B_1 \\ 0 & A_2 & B_2 \end{bmatrix}$$

where the A_i contains nonzero components of equations corresponding to coordinates of the interior stations in \mathcal{A}_i and where the B_i contain the nonzero components of equations corresponding to the coordinates of the stations in the junction region B .

Next, in each of these halves we pick a longitude so that approximately one-half of the stations in that region lie to the east of that longitude. This constitutes level 2 of nested bisection. The process can then be continued by successively subdividing the smaller regions, alternating between latitudinal and longitudinal dividing lines. Figure 4 illustrates three levels

of nested bisection.

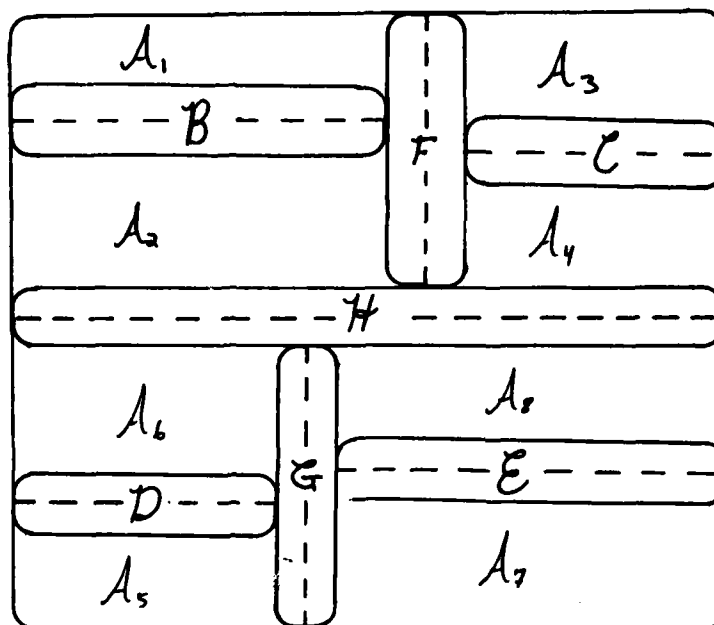
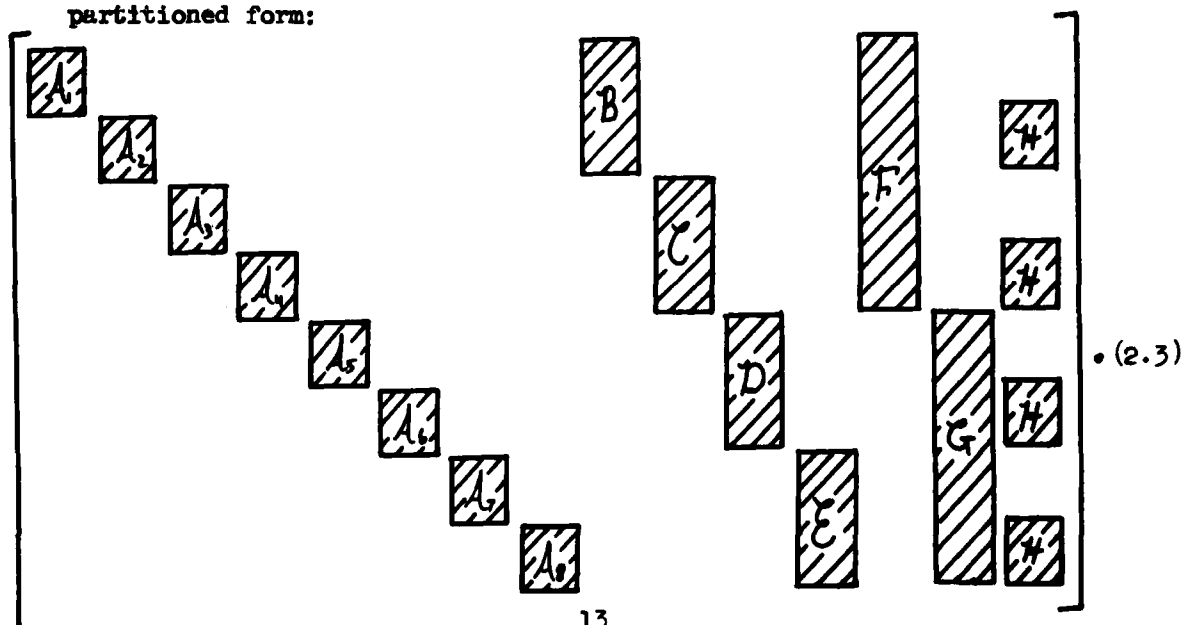


FIGURE 4

Three levels of nested bisection.

The observation matrix associated with the nested bisection of the geodetical position network in Figure 4 can then be assembled into the partitioned form:



It follows that if nested bisection is carried out to k levels, then the partitioned form of the assembled observation matrix has:

- i) 2^k diagonal blocks associated with interior regions, and
- ii) 2^{k-1} blocks associated with junction regions.

In particular, there are

- iii) 2^{k-1} junction blocks which are each coupled to 2 interior regions, and
- iv) $2^{k-1}-1$ junction blocks which are each coupled to 4 interior regions.

Heuristically, one normally would like to perform the bisection process so that the sets of junction stations are minimal at each level, thus maximizing the numbers of columns in the diagonal blocks. The process is stopped at the level k at which the 2^k diagonal blocks are sufficiently dense or at the level at which further subdivisions are not feasible or are not necessary for the particular adjustment problem.

Our proposed block orthogonal decomposition algorithm for an observation matrix A already in the partitioned form determined by nested bisection is deferred to the next section.

3. The Block Orthogonal Decomposition.

In this section we describe a block orthogonal decomposition algorithm for solving the least squares adjustment problem $\min_x \|b - Ax\|_2$, where the observation matrix A has been assembled into the general block diagonal form (1.4). Here we assume that the structure of A is specified by the nested bisection scheme described in Section 2. Other dissection

schemes may be preferable in certain applications (see Golub and Plemmons [1980]).

We first illustrate the method with $k = 2$ levels of nested bisection, as given in Figure 5.

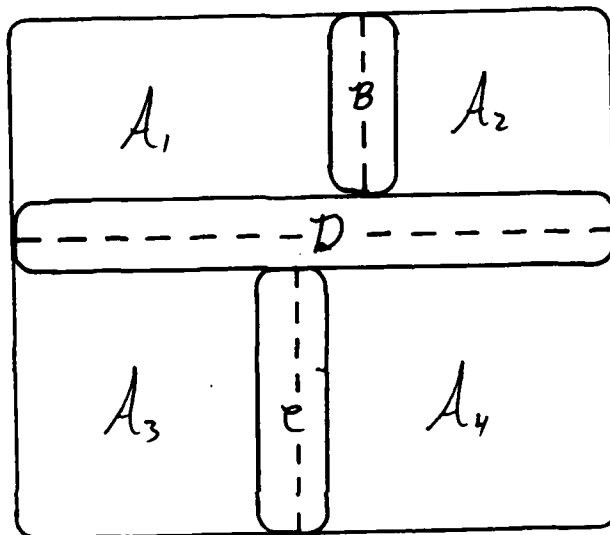


FIGURE 5

Two levels of nested bisection.

Suppose that the associated observation matrix A is assembled into the corresponding block-partitioned form, giving

$$A = \begin{bmatrix} A_1 & & & B_1 & D_1 \\ & A_2 & & B_2 & D_2 \\ & & A_3 & & C_3 & D_3 \\ & & & A_4 & C_4 & D_4 \end{bmatrix}$$

Then by the use of orthogonalization techniques based upon, for example, Householder reflections, Givens rotations or modified Gram-Schmidt orthogonalization, the reduction of A to upper triangular form proceeds as follows:

At the first stage, each diagonal block A_i is reduced by orthogonal transformations.

$$\begin{matrix} Q_1^t \rightarrow \\ Q_2^t \rightarrow \\ Q_3^t \rightarrow \\ Q_4^t \rightarrow \end{matrix} \begin{bmatrix} A_1 & & B_1 & D_1 \\ & A_2 & B_2 & D_2 \\ & & A_3 & C_3 & D_3 \\ & & & A_4 & C_4 & D_4 \end{bmatrix}$$

Here the Q_i are orthogonal matrices (which of course need not be formed explicitly) and $Q_i^t A_i = \begin{bmatrix} R_i \\ 0 \end{bmatrix}$, where $R_i = \begin{bmatrix} \text{upper triangular} \\ 0 \end{bmatrix}$, yielding

$$\begin{bmatrix} R_1 & & B_1^0 & D_1^0 \\ 0 & & B_1^1 & D_1^1 \\ & R_2 & B_2^0 & D_2^0 \\ & 0 & B_2^1 & D_2^1 \\ & & R_3 & C_3^0 & D_3^0 \\ & & 0 & C_3^1 & D_3^1 \\ & & & R_4 & C_4^0 & D_4^0 \\ & & & 0 & C_4^1 & D_4^1 \end{bmatrix}$$

The row blocks corresponding to the upper triangular matrices R_i are then merged through a permutation of the rows, yielding

$$\begin{matrix} Q_5^t \rightarrow \{ \\ Q_6^t \rightarrow \{ \end{matrix} \left[\begin{array}{ccccccc} R_1 & & & & B_1^0 & & D_1^0 \\ & R_2 & & & B_2^0 & & D_2^0 \\ & & R_3 & & & C_3^0 & D_3^0 \\ & & & R_4 & & C_4^0 & D_4^0 \\ & & & & B_1^1 & & D_1^1 \\ & & & & B_2^1 & & D_2^1 \\ & & & & & C_3^1 & D_3^1 \\ & & & & & C_4^1 & D_4^1 \end{array} \right]$$

This completes the first stage of the reduction. For the intermediate stages, pairs of merged blocks corresponding to junction stations are reduced. First, $\begin{bmatrix} B_1^1 \\ B_2^1 \end{bmatrix}$ and $\begin{bmatrix} C_3^1 \\ C_4^1 \end{bmatrix}$ are reduced to upper triangular form by orthogonal transformations, yielding

$$\left[\begin{array}{ccccccc} R_1 & & & & B_1^0 & & D_1^0 \\ & R_2 & & & B_2^0 & & D_2^0 \\ & & R_3 & & & C_3^0 & D_3^0 \\ & & & R_4 & & C_4^0 & D_4^0 \\ & & & & R_5 & & D_5^0 \\ & & & & 0 & & D_5^1 \\ & & & & & R_6 & D_6^0 \\ & & & & & 0 & D_6^1 \end{array} \right]$$

Then merging the triangular factors R_5 and R_6 through a permutation of the rows, yields

$$Q_7^t \rightarrow \left[\begin{array}{cccccc} R_1 & & & & B_1^0 & D_1^0 \\ & R_2 & & & B_2^0 & D_2^0 \\ & & R_3 & & C_3^0 & D_3^0 \\ & & & R_4 & C_4^0 & D_4^0 \\ & & & & R_5 & D_5^0 \\ & & & & & R_6 & D_6^0 \\ & & & & & & D_5^1 \\ & & & & & & D_5^1 \\ & & & & & & D_6^1 \end{array} \right]$$

To complete the intermediate stages, $\left[\begin{array}{c} 1 \\ D_5^1 \\ D_6^1 \end{array} \right]$ is reduced to upper triangular form by orthogonal transformations, yielding

$$R = \left[\begin{array}{cccccc} R_1 & & & & B_1^0 & D_1^0 \\ & R_2 & & & B_2^0 & D_2^0 \\ & & R_3 & & C_3^0 & D_3^0 \\ & & & R_4 & C_4^0 & D_4^0 \\ & & & & R_5 & D_5^0 \\ & & & & & R_6 & D_6^0 \\ & & & & & & R_7 \end{array} \right]$$

Here R is the Cholesky factor for A . Let n_i denote the order of R_i for $i = 1, \dots, 7$ and let $c^t = (c_1, \dots, c_7)^t$ denote the result of applying the same sequence of orthogonal transformations and permutations to b , where each c_i is an n_i -vector. For the final step of the solution process, the least squares solution y to $Ax \approx b$ is computed as follows.

Partition y as $y^t = (y_1, \dots, y_7)^t$ where y_i is an n_i -vector, $i = 1, \dots, 7$. Then the following upper triangular systems are solved successively by back-substitution for the vectors y_i , $i = 7, 6, \dots, 1$.

$$R_7 y_7 = c_7,$$

$$R_i y_i = c_i - D_i^0 y_7, \quad i = 6, 5,$$

$$R_i y_i = c_i - C_i^0 y_6 - D_i^0 y_7, \quad i = 4, 3,$$

$$R_i y_i = c_i - B_i^0 y_5 - D_i^0 y_7, \quad i = 2, 1.$$

The general reduction process is described next in terms of three basic steps. Let A and b denote the observation matrix and vector resulting from k levels of nested bisection of a geodetic position network on some geographical region. Assume that A has been assembled into the general block-partitioned form (1.4), with 2^k diagonal blocks and $2^k - 1$ remaining column blocks. Letting $t = 2^k$, we write A as

$$A = \begin{bmatrix} A_1 & & & & A_{1,t+1} & \cdot & \cdot & \cdot & A_{1,2t-1} \\ & A_2 & & & A_{2,t+1} & \cdot & \cdot & \cdot & A_{2,2t-1} \\ & & \cdot & & \cdot & & & & \cdot \\ & & & \cdot & \cdot & & & & \cdot \\ & & & & \cdot & & & & \cdot \\ & & & & A_t & A_{t,t+1} & \cdot & \cdot & A_{t,2t-1} \end{bmatrix} \quad (3.1)$$

For a certain flexibility of the algorithm and also for simplicity in the notation, we do not altogether distinguish here between zero and nonzero blocks A_{ij} . The zero pattern of these blocks depends on the number of levels, k , to which the nested bisection process is carried. Particular attention was paid to this pattern for the case of $k = 2$ levels in the illustrative example just completed.

Algorithm 1. This algorithm computes the Cholesky factor R and the least squares solution y to $Ax \approx b$ where A results from k levels of nested bisection and A has the block form (3.1), with $t = 2^k$.

Step 1. Reduce each diagonal block A_i of A to upper triangular form by orthogonal transformations and merge the reduced blocks.

1) Do for $i = 1, 2, \dots, t$.

1) Determine Q_i^t so that $Q_i^t A_i = \begin{bmatrix} R_i \\ 0 \end{bmatrix}$, $R_i = \begin{bmatrix} \text{upper triangular} \\ 0 \end{bmatrix}$
 (Note that Q_i^t need not be formed explicitly).

2) Compute

$$Q_1^t[A_1, A_{1,t+1}, \dots, A_{1,2t-1}]$$

$$= \begin{bmatrix} R_1 & A_{1,t+1}^0 \dots A_{1,2t-1}^0 \\ 0 & A_{1,t+1}^1 \dots A_{1,2t-1}^1 \end{bmatrix}$$

2) Merge the reduced row blocks by row permutations so that the resulting matrix has the form

$$\begin{bmatrix} R_1 & A_{1,t+1}^0 & A_{1,t+2}^0 & \dots & A_{1,3t/2}^0 & A_{1,(3t/2)+1}^0 & \dots & A_{1,2t-1}^0 \\ R_2 & A_{2,t+1}^0 & A_{2,t+2}^0 & \dots & A_{2,3t/2}^0 & A_{2,(3t/2)+1}^0 & \dots & A_{2,2t-1}^0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ R_t & A_{t,t+1}^0 & A_{t,t+2}^0 & \dots & A_{t,3t/2}^0 & A_{t,(3t/2)+1}^0 & \dots & A_{t,2t-1}^0 \\ & A_{1,t+1}^1 & & & & A_{1,(3t/2)+1}^1 & \dots & A_{1,2t-1}^1 \\ & A_{2,t+1}^1 & & & & A_{2,(3t/2)+1}^1 & \dots & A_{2,2t-1}^1 \\ & & A_{3,t+2}^1 & & & A_{3,(3t/2)+1}^1 & \dots & A_{3,2t-1}^1 \\ & & A_{4,t+2}^1 & & & A_{4,(3t/2)+1}^1 & \dots & A_{4,2t-1}^1 \\ & & & \dots & & \dots & \dots & \dots \\ & & & & A_{t-1,3t/2}^1 & A_{t-1,(3t/2)+1}^1 & \dots & A_{t-1,2t-1}^1 \\ & & & & A_{t,3t/2}^1 & A_{t,(3t/2)+1}^1 & \dots & A_{t,2t-1}^1 \end{bmatrix}$$

Step 2. Reduce and merge the intermediate-stage blocks.

1) Do for $u = t, t/2, \dots, t/2^{k-1} = 2$.

1) Do for $v = 1, 3, \dots, u-1$

1) Reduce each pair of row diagonal blocks

$$\begin{bmatrix} A_{v,t+v}^1 \\ A_{v+1,t+v}^1 \end{bmatrix}$$

to upper triangular form by orthogonal transformation,
as in Step 1.

2) Merge the resulting reduced row blocks by row permutations
so that the upper triangular blocks R_i appear first, as
in Step 1.

At the end of Step 2, A has been reduced by orthogonal transformations
to the following form, where each R_i is upper triangular and where certain
of the blocks A_{ij}^0 are zero.

$$R = \begin{bmatrix} R_1 & & & A_{1,t+1}^0 & \cdot & \cdot & \cdot & A_{1,2t-1}^0 \\ & R_2 & & A_{2,t+1}^0 & \cdot & \cdot & \cdot & A_{2,2t-1}^0 \\ & & \cdot & \cdot & & & & \cdot \\ & & & \cdot & & & & \cdot \\ & & & \cdot & & & & \cdot \\ & & & R_t & A_{t,t+1}^0 & \cdot & \cdot & A_{t,2t-1}^0 \\ & & & & R_{t+1} & & & \cdot \\ & & & & & \cdot & & \cdot \\ & & & & & & \cdot & \cdot \\ & & & & & & & A_{2t-2,2t-1}^0 \\ & & & & & & & R_{2t-1} \end{bmatrix} \quad (3.2)$$

Step 3. Back Substitution. Let n_i denote the order of R_i , for $i = 1, \dots, 2t-1$. Let $c^t = (c_1, \dots, c_{2t-1})^t$ denote the result of applying the same sequence of orthogonal transformations to b and let $y^t = (y_1, \dots, y_{2t-1})^t$ denote the least squares solution to $Ax \approx b$, where c_i and y_i are n_i -vectors, $i = 1, \dots, 2t-1$. Solve each of the following upper-triangular systems by back-substitution

$$1) \quad R_{2t-1} y_{2t-1} = c_{2t-1}$$

$$2) \quad R_i y_i = c_i - \sum_{j=i+1}^{2t-1} A_{ij}^0 y_j, \quad i = 2t-2, 2t-1, \dots, t$$

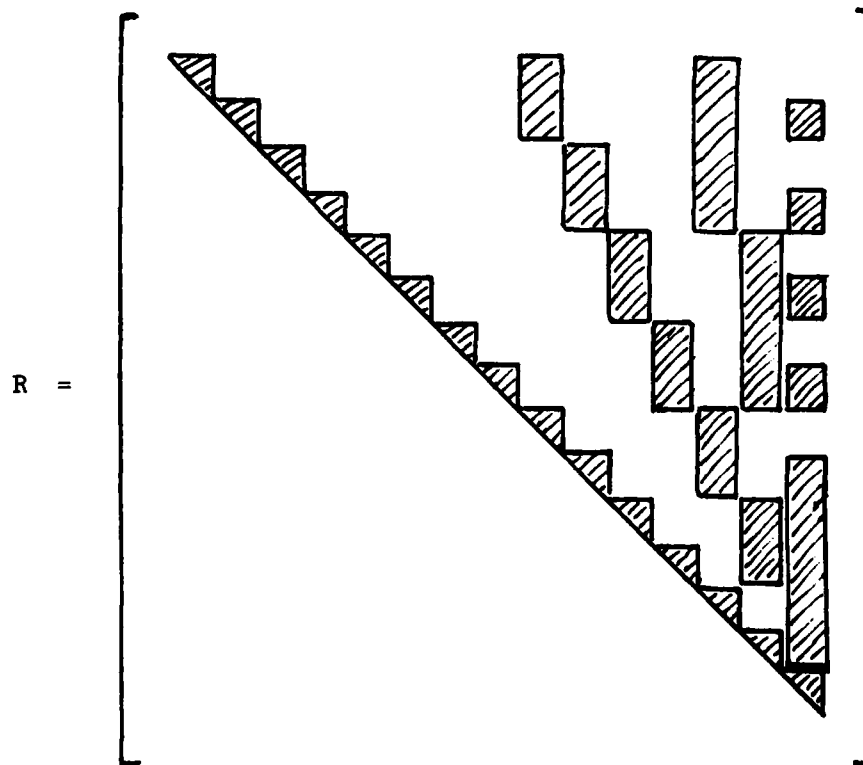
$$3) \quad R_i y_i = c_i - \sum_{j=t+1}^{2t-1} A_{ij}^0 y_j, \quad i = t, t-1, \dots, 1.$$

The reduction algorithm just described for the observation matrix A can be interpreted from a network-reduction viewpoint as follows. Suppose that A results from a nested bisection of the geographical region to k levels. Then at the first stage of the reduction process, orthogonal transformations are applied to each of the 2^k blocks corresponding to the interior regions, to reduce the coordinates of stations not coupled to stations outside that block by an observation. Modified junction stations in the separator blocks are kept until nearby interior blocks are reduced. Then clusters of blocks of junction stations are grouped together (merged) to form higher level blocks. At the intermediate stages of the reduction process, some station coordinates are now interior and can be reduced by orthogonal transformations. The process continues until at the last stage the remaining stations are all interior and their coordinates can be reduced. At this point A is completely reduced by orthogonal transformations to its Cholesky factor R , and correspondingly, the vector b is reduced to c as indicated in Step 3. To determine the least squares solution y to $Ax \approx b$, the process is, in a sense, reversed to back substitute the coordinates to successively lower levels until all of the corrections have been found.

Notice that at each stage of the reduction process it is possible to obtain a "diagnostic solution" (see Meissl [1979]). Here we hold the coordinates of the junction stations fixed and solve for the coordinates of the reduced interior stations at that stage.

We emphasize again that, for a certain flexibility, full advantage has

not been taken in Algorithm 1 of the zero pattern of the blocks A_{ij} of A as given by (3.1). This pattern of course determines the block structure of the Cholesky factor R of A as given by (3.2). Basically, R has the same type of block structure as A , but with $2^{k+1}-1$ upper-triangular diagonal blocks. For nested bisection to $k = 4$ levels, where A is assembled into the form (2.3), the Cholesky factor R has the following structure.



In order to facilitate an analysis of the results of a least squares adjustment, it is often desirable to compute some or all of the elements of the variance-covariance matrix $(A^t A)^{-1}$. Since

$$(A^t A)^{-1} = (R^t R)^{-1} ,$$

the special block structure of R just discussed can be used advantageously in computing the variances and covariances. Such a procedure is given in the next section for a more generally sparse Cholesky factor R .

4. Computation of the Variances.

In many adjustment problems (see, for example, Hanson [1978]) it is necessary to compute the variances and covariances associated with the regression coefficients in order to estimate the accuracy of the results. Under the usual assumptions, the variance of the i -th coefficient is proportional to the (i,i) element of $(A^t A)^{-1}$. If R is sparse, then the diagonal elements of $(A^t A)^{-1}$ can be calculated quite efficiently. Indeed, it is easy to compute all the elements of $(A^t A)^{-1}$ which are associated with the non-zero elements of R , the Cholesky factor. We describe the procedure next.

Using the orthogonalization algorithm we determine the Cholesky factor R so that

$$A^t A = R^t R .$$

Suppose

$$\begin{aligned} r_{ij} &\neq 0 && \text{when } (i,j) \in K \\ &= 0 && \text{when } (i,j) \notin K . \end{aligned}$$

Our objective is to determine

$$\{(A^t A)^{-1}\}_{ij} \quad \text{When } (i,j) \in K.$$

Let us write

$$(A^t A)^{-1} = Z = [z_1, \dots, z_n],$$

where z_i is the i -th column of the matrix Z .

Since

$$\begin{aligned} A^t A Z &= I \\ R Z &= (R^t)^{-1}. \end{aligned} \tag{4.1}$$

Note that

$$\{(R^t)^{-1}\}_{ii} = 1 / r_{ii}. \tag{4.2}$$

From (4.1) and (4.2), we see that

$$R z_n = e_n \times (r_{nn})^{-1} \quad (e_n^t = (0, \dots, 0, 1))$$

so that we can solve for z_n by back substitution. Thus

$$z_{nn} = (r_{nn})^{-2}$$

and for $i = n-1, n-2, \dots, 1$

$$z_{in} = \sum_{j=i+1}^n \frac{r_{ij}}{r_{ii}} z_{jn} = \sum_{\substack{j=i+1 \\ (i,j) \in K}}^n \frac{r_{ij}}{r_{ii}} z_{jn}.$$

Let $I_n = \min_{1 \leq i \leq n-1} \{i \mid r_{in} \neq 0\}$. It is possible to calculate z_{in} for $i = n-1, n-2, \dots, I_n$. Once these components have been computed, it is only necessary to save those elements for which $(i, n) \in K$.

Note

$$z_{in} = z_{ni}.$$

Now assume we have calculated those elements of $z_n, z_{n-1}, \dots, z_{l+1}$ for which

$$r_{pq} \neq 0 \quad \text{when} \quad p=1, \dots, n; \quad q = l+1, \dots, n.$$

Thus, by symmetry we have computed

$$z_{ql} \quad \text{for} \quad q > l \quad \text{and} \quad (l, q) \in K.$$

Now for $i = 1, 2, \dots, l-1$

$$\sum_{j=i}^n r_{ij} z_{jl} = 0$$

and

$$\sum_{j=l}^n r_{lj} z_{jl} = \frac{1}{r_{ll}}.$$

Hence

$$\begin{aligned} z_{ll} &= \frac{1}{r_{ll}} \left(\frac{1}{r_{ll}} - \sum_{j=l+1}^n r_{lj} z_{jl} \right) \\ &= \frac{1}{r_{ll}} \left(\frac{1}{r_{ll}} - \sum_{\substack{j=l+1 \\ (l,j) \in K}}^n r_{lj} z_{jl} \right) \end{aligned}$$

Let $I_l = \min_{1 \leq i \leq l-1} \{i \mid r_{il} \neq 0\}$. Then for $i = l-1, \dots, I_l$

$$z_{il} = \left(- \sum_{\substack{j=i+1 \\ (i,j) \in K}}^l r_{ij} z_{jl} - \sum_{\substack{j=l+1 \\ (i,j) \in K}}^n r_{ij} z_{lj} \right) / r_{ii}.$$

Again, after this calculation is performed, we save only those elements for which $(i,l) \in K$. The above algorithm thus describes a method for computing the elements of the inverse of $(A^t A)$ which are associated with the non-zero elements of R . Such a procedure can be quite efficient when compared to computing

$$(A^t A)^{-1} = R^{-1} (R^t)^{-1}.$$

For example, suppose we need the diagonal elements of $(A^t A)^{-1}$ when

$$r_{ij} \neq 0 \quad \text{for } i = j \quad \text{and } j = i+1, \text{ and}$$

$$r_{ij} = 0 \quad \text{otherwise,}$$

i.e. R is bi-diagonal. The matrix R^{-1} will be completely filled in above the diagonal and hence $O(n^2)$ numerical operations are required to compute the diagonal elements of $(A^t A)^{-1}$. The algorithm we have outlined above would require $O(n)$ operations. Even greater savings can be expected for the Cholesky factor R of the form (3.2), resulting from nested bi-section.

5. Final Remarks.

To summarize, an alternative has been provided here to the formation and solution of the normal equations in least squares adjustment problems. In particular, it has been shown how a block-orthogonal decomposition method

can be used in conjunction with a nested dissection scheme to provide a least squares algorithm for certain geodetic adjustment problems.

Some well-known advantages of dissection schemes for sparse linear systems are that they facilitate efficient data management techniques, they allow for the use of packaged matrix decomposition routines for the dense component parts of the problem, and they can allow for the use of parallel processing. In the past, the combination of the normal equations approach with these dissection techniques (in particular Helmert blocking) has been preferred, partly because of tradition and partly because of the simplicity and numerical efficiency of the Cholesky decomposition method. However, the use of an orthogonal decomposition scheme applied directly to an observation matrix A which has also been partitioned by a dissection scheme has several advantages over the normal equations approach. First, the QR orthogonal decomposition of A allows for an efficient and stable method of adding observations to the data (See Gill, Golub, Murray and Saunders [1974]). Such methods are crucial in certain large-scale adjustment problems (see Hanson [1978]). Secondly, possible fill-in that can occur in forming the normal equation matrix $A^t A$ is avoided. A statistical study of such fill-in is provided by Bjorck [1976]. Meissl [1979] reports that some fill-in can be expected in forming $A^t A$ in the readjustment of the North American Datum. This problem cannot be over-emphasized in such large scale-systems (6,000,000 equations and 400,000 unknowns). But perhaps the most crucial advantage of the use of orthogonal-decomposition schemes here is that they may reduce the effects of ill-conditioning in adjustment calculations.

In this paper we have treated only one aspect of nested dissection in least squares problems, that of decomposing a geodetical position network by the process of nested bisection. However, the block diagonal form of the matrix in (1.4) can arise in other dissection schemes such as one-way dissection (see George, Poole and Voight [1978] for a description of this scheme for solving the normal equations associated with finite element problems). The form also arises in other contexts, such as photogrammetry (See Golub, Luk and Pagano [1979]). Least squares schemes based in part upon block iterative methods (see Plemmons [1979]) or a combination of direct and iterative methods may be preferable in some applications. Moreover, the general problem of permuting A into the form (1.4) by some graph-theoretic algorithm for ordering the rows and columns of A (see Weil and Kettler [1971]) has not been considered in this paper. Some of these topics will be addressed further in Golub and Plemmons [1980].

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